

On the importance of grain boundaries in HT_c films: simulation results

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Abstract

The importance of the distribution and “weakness” of grain boundary junctions in the magnetic field dependence of the transport critical current in HT_c films is assessed through simulations. The system is studied with the applied field either parallel or perpendicular to the \vec{c} axis of the sample. For *realistic* sample parameters, it is demonstrated that the presence of “high” misorientation angles between grains depresses the zero - field critical current density in both orientations, and provokes a transition from pinning-mediated to Fraunhofer-like field dependencies of the critical current density. Our results also suggest that there is a threshold misorientation angle above which the critical current density remains constant.

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1 Introduction

One of the limiting factors found in the race to get large scale applications from HT_c superconductors is their granular character which constitutes a severe handicap to obtain large values of critical current densities.

From today's variety of HT_c superconducting materials, bismuth tapes seem to be the best solution when we are looking for good mechanical properties and low cost performance figures (see for example [1] and [2]). However, the highest values of critical current densities are obtained in $YBaCuO$ thin films, so this material cannot be discarded as a possibility for current carrying applications [3].

It is generally observed that these thin films grow through a nucleation process resulting in "islands" or "columnar grains" [4, 5]. The existence and nature of weak links between these columnar grains have been the subject of debate for years since they are strongly dependent on the deposition technique, the substrate, and deposition parameters. However, there is a general agreement that in thin films, contrary to what happens in ceramic superconductors, transport properties are dominated by pinning mechanisms instead of Josephson effects.

In spite of this general belief, a great fraction of the published data in the field shows the presence of low and large angle boundaries between grains in HT_c films, (particularly polycrystalline), and at the same time, careful studies of Chaudhary et al [6] and Gross [7] demonstrated that high angle grain boundaries drastically reduce the critical current of the junctions. To clarify the role of those boundaries, and of the pinning centers on the resulting critical current density, we developed a simple model for the transport properties of thin film superconductors.

2 The Model

The critical current density within each superconducting grain is assumed to change with the field following a Kim-like model [8] as:

$$J_{ci} \sim \frac{1}{1 + H/H_o} \quad (1)$$

where the subscript ci stands for the different directions of the current (x, y, z), H is the magnetic field applied to the sample, and H_o is a parameter to be determined experimentally.

This equation can be written in the following more convenient form for computational purposes:

$$J_{ci} \sim \frac{1}{1 + \beta p} \quad (2)$$

where p represents a normalized magnetic field, and β is a parameter which depends on the relation between the field orientation and the sample axis. Following figure 1, the values of β considered were: if \vec{H}/\vec{c} , $\beta = 1$ for J_{cx} and J_{cz} and $\beta = 0$ for J_{cy} ; if $\vec{H} \perp \vec{c}$ (\vec{H} along \vec{x}), $\beta = 0.1$ for J_{cz} , $\beta = 1.0$ for J_{cy} and $\beta = 0$ for J_{cx} . To choose these values, we assumed that the intragranular current was depressed only by magnetic fields perpendicular to the current flow, and that the intrinsic pinning (i.e. that acting on the vortices lying parallel to the ab planes when forced to move perpendicular to them) was an order of magnitude stronger than other sources of pinning [9, 10].

Up to this point, the model describes the field dependance of the critical current density in an *homogeneous* medium (i.e., not *weak* links between grains). However, if between the grains of the thin film high angle tilt boundaries exist, the problem becomes more complicated. In fact, if between two grains a high angle tilt boundary exists, the *intergranular* critical current density follows the well-known Fraunhofer pattern for a short Josephson junction [11]:

$$A \frac{\sin(\pi \frac{\Phi}{\Phi_o})}{\pi \frac{\Phi}{\Phi_o}} \quad (3)$$

where the prefactor A depends on the angle boundary, Φ is the magnetic flux at the junction, and Φ_o is the flux quantum.

Now, we can rewrite (3) as a function of $p = H/H_o$, and, after a straightforward algebra, it is transformed in:

$$A \frac{\sin(\alpha p)}{\alpha p} \quad (4)$$

where $\alpha = \pi \frac{d\lambda H_o}{\Phi_o}$ for \vec{H}/\vec{c} and $\alpha = \pi \frac{L\lambda H_o}{\Phi_o}$ for $\vec{H} \perp \vec{c}$, (d and L are represented in figure 1).

A granular thin film can not be modeled as a pure ceramic superconductor since, having just a small fraction of high angle tilt boundaries, we can find paths of high critical current densities where its dependence with the applied field is determined by the equation (2). So, to model the system we proposed a tridimensional array of grains, a fraction q of them was strongly coupled (which means with misorientation angle smaller than 7° occur between grains [4]), while a fraction $(1 - q)$ is coupled through weak links produced by high angles between grains. For the strongly coupled grains the critical current

density was determined by means of (2), while for the weakly coupled grains equation (4) was used.

The calculation of the critical current density of the system was based on the Minimum Cut Algorithm already used to solved similar problems [14, 15]. This algorithm allows the calculation of the maximum flow in a random system. It is basically composed by two operations. A first one to determine the paths on the system where the current can flow, and a second one to augment the flow (of current) at the bonds (our links between grains). Once it is impossible to find a new path or to augment the flow through the already found paths, we say we obtained the maximum current (critical current) of the system.

We choose for our simulations $\alpha = 20$ for \vec{H}/\vec{c} which corresponds to $L = 600nm$ and $\lambda = 30nm$, and $\alpha = 400$ for $\vec{H} \perp \vec{c}$ corresponding to $d = 200nm$ and $\lambda = 200nm$ as typically reported for *YBaCuO* films (see figure1) [4, 5]. Kim's characteristic field $H_o = 1T$ was assumed. The possibility of modeling granularity in such anisotropic fashion (but only in the light of a simple parallel ensemble of Josephson junctions) has been suggested earlier by Altshuler et al [12]. We used systems of dimensions $16 \times 16 \times 16$ (which mimics a $\sim 10 \times 10 \mu m^2$ bridge performed on a thin film with average grain diameter of $600nm$) and averaged over 10 different configurations to improved the statistics. The parameter p was always varied between 0 and 3.

One more remark about the different configurations used is needed. If the applied field points parallel to the \vec{c} direction, junctions perpendicular to the *ab* plane (shaded in figure 1) are affected by equation (4), while, if it is applied parallel to the *ab* plane, junctions lying in that plane are not affected.

3 Results

To approach real values of *YBaCuO* films we extracted A and q from the combination of two experimental results: the statistics of boundaries angles in a *YBaCuO* films reported by [4], and the angle dependence of the critical current density measured by Ivanov et al [16] on *YBaCuO* bycrystals. Figure 2 shows the simulated field dependence of the critical current density corresponding to films with different microstructures. The upper curve represents the critical current versus field dependence of a system without weak-links, while the lower contains a 50% of high angle boundaries. 80% and 20%

of these boundaries reduce the critical current by approximate factors of 2 and 100 respectively, corresponding to misorientation angles of 8° and 20° [4, 16]. As observed in figure 2 the introduction of weak-links provokes a reduction of the zero field critical current density by a factor 0.67. It also induces a steeper $J_c(p)$ characteristic in the “low field” region, and several maxima which suggests a superposition of Josephson patterns, as observed in *YBaCuO* polycrystals with a small number of grains [17, 18].

To model a better sample, we calculated J_c for a system without boundaries reducing the critical current by a factor 100. The results are shown in figure 3, where the critical current density as a function of p is plotted for a set of systems with q ranging from 0.50 to 1.0. Even in this case the critical current density depends on the number of weak-links. However, interestingly enough, the suppression of the “worst” boundaries doesn’t improve significantly the critical current density at zero field. This suggests that the number of weak-links is more important than their “weakness” regarding the absolute values of the critical current.

To further explore this idea in figure 4, we compared the critical current dependencies with the applied field of samples with different kinds of weak-links and $q = 0.5$. The upper curve represents angles in the range $7^\circ - 10^\circ$, i.e. reducing J_c by a factor of 2, while the remaining curves represent angles of $12^\circ, 15^\circ, 25^\circ$ and 40° which roughly reduce the critical current by 4, 10, 100 and 10000 respectively [4, 16]. The figure shows again similar J_c vs p dependencies for high values of the angles. For high fields all the curves behave in the same manner, indicating that, in this regime, the number of weak links is more important than their quality. However, for zero field, different values of critical current densities are obtained depending on the misorientation angle between grains. Figure 5 shows this dependence, demonstrating that angles greater than 25° , do not considerably change the critical current densities values, while a strong improvement in J_c can be obtained by diminishing the angle below 25° , which is qualitatively coherent with the data of Wu et al [19].

Figure 6 shows the field dependence of the critical current density for the $\vec{H} \perp \vec{c}$ configuration. When compared with the figure 3, the effect of an anisotropic set of parameters is revealed in a less strong field dependence of J_c . However, the depression in the zero field critical current density is roughly similar to the $\vec{H} // \vec{c}$ configuration. Here the weak-linked component also introduces a steep $J_c(p)$ characteristics in the “low field” region, while Josephson assembly-like maxima are observed as q decreased.

4 Conclusions

From these results we conclude that the presence of high angle boundaries reduces the critical current density of superconducting thin films and provokes a transition from pinning-mediated to Fraunhofer-like patterns in its magnetic field dependencies. Our results also suggest that the amplitude of the misorientation angles between grains *does not* change the values of critical current density for high values of the applied field, while for low applied field, differences appear only for small angle values.

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Figure Captions

Figure 1 Diagram of the system used in our simulations

Figure 2 J_c vs p dependences for $\vec{H} // \vec{c}$. Upper curve: $q=1$, Bottom curve: $q=0.5$. Two qualities of high misorientation angles, $A = 0.5$ and $A = 0.001$

Figure 3 J_c vs p dependences for $\vec{H} // \vec{c}$. From top to bottom: $q = 1, 0.8, 0.7$ and 0.5 . One quality of high misorientation angles, $A = 0.5$

Figure 4 J_c vs p dependences, $\vec{H} // \vec{c}$, $q = 0.5$. From top to bottom: $A = 0.5, 0.25, 0.1, 0.01$ and 0.0001 correspondig to misorientation angles of $7^\circ < \theta < 10^\circ, 15^\circ, 25^\circ$ and 40° .

Figure 5 J_c dependence with the approximate misorientation angle, $q = 0.5$

Figure 6 J_c vs p dependences, $\vec{H} \perp \vec{c}$. From top to bottom $q = 1, 0.8, 0.7$ and 0.5











